NASA Conference Publication 2136

Review of Spectroscopic Data for Measurements of Stratospheric Species

Proceedings of a workshop held at
NASA Langley Research Center
Hampton, Virginia
October 29-30, 1979

NASA

NASA Conference Publication 2136

Review of Spectroscopic Data for Measurements of Stratospheric Species

Editors
Aaron Goldman, *University of Denver*
James Hoell, *Langley Research Center*

Proceedings of a workshop sponsored by NASA Langley Research Center, Hampton, Virginia, and held at Langley Research Center October 29-30, 1979

NASA
National Aeronautics and Space Administration

Scientific and Technical Information Office

1980

PREFACE

This conference publication contains the proceedings of a workshop on October 29-30, 1979, at Langley Research Center. The workshop was a review of the status of infrared spectroscopic data and as such was a follow-up of work begun at the workshop on High Resolution Infrared Spectroscopy Techniques for Upper Atmospheric Measurements held in Silverthorne, Colorado, on July 31 to August 2, 1979. (Available as NASA CP-2134.) The proceedings presented herein also appear as appendix 4 in the proceedings of the Silverthorne conference. The workshop held at Langley was chaired by Aaron Goldman from the University of Colorado and by James M. Hoell of Langley. A list of attendees is included.

The objectives of this workshop were to review in detail the current status of experimental and theoretical spectroscopic data on atmospheric species, to explore methods for disseminating new data in a format readily available for applications, and to discuss formalization of the workshop in order to support the first two objectives on a long term basis. As a result of this workshop, plans were made to establish a periodic newsletter and to hold at least one more meeting to keep individuals up to date on the progress of research involving spectral data.

INTRODUCTION

Background

Under NASA's Upper Atmospheric Research Program (UARP) a wide range of infrared instruments have been developed or are in various states of development for atmospheric research from Shuttle or free flyer platforms. These instruments encompass a range of spectral resolution (i.e., from 0.1 cm^{-1} to less than 0.001 cm^{-1}) and spectral coverage (i.e., from several hundred cm^{-1} to less than 0.001 cm^{-1}). The "Workshop on High Resolution Infrared Spectroscopy Techniques for Upper Atmospheric Measurements" held in Silverthorne, Colorado, July 31 to August 2, 1979, was convened to assess the role of various infrared techniques in measurements of trace gases in the stratosphere. The Workshop placed particular emphasis on the role of instruments exhibiting ultrahigh resolution (i.e., $\lesssim$0.001 cm^{-1}) such as laser heterodyne spectrometers. The Workshop brought together scientists engaged in laboratory and upper atmosphere high resolution infrared spectroscopy. The participants were organized into four working groups, one of which considered the status of infrared spectroscopic data. The spectroscopic workshop, which will be discussed below, is a direct result of the general discussions held at Silverthorne and specific recommendations from the spectroscopic working group at Silverthorne.

At the Silverthorne Workshop, it was generally recognized that current and future stratospheric measurements as well as evaluation of the relative merits of the various instruments depends heavily upon the availability and accuracy of infrared spectroscopic data for all stratospheric species. The Workshop noted that a large body of spectroscopic data is currently available, particularly for the more abundant atmospheric species (i.e., CO_2, O_3, CH_4, N_2O, and H_2O). However, for many trace species currently of interest (ClO, $ClONO_2$, HO_2, H_2O_2, etc.) little, if any, data are available. Furthermore, it was noted that additional experimental and theoretical research is needed for virtually all species to support the high resolution instruments becoming available. The Silverthorne Workshop also noted the limitation of the spectroscopic data base which is widely used by many groups (i.e., A.F. Geophysics Laboratory (AFGL) tape). This tape, while extremely useful, is inadequate for many high resolution applications. Because of this, many laboratories in the United States and foreign countries have, or are in the process of, improving the spectral data on the AFGL tape; however, the availability and format of this data is such that it is not readily available to the community.

From these general observations, the Silverthorne spectroscopic working group recommended that a detailed review of the current spectroscopic data base be conducted and that a formalized mechanism be established to facilitate dissemination of existing and future spectroscopic data to the appropriate users. To this end, the spectroscopic working group from Silverthorne was reconvened at the Langley Research Center as an informal workshop with wider representation from various U.S. and foreign spectroscopic laboratories.

Scope of Spectroscopic Workshop

The first meeting was held October 29-30, 1979, at Langley Research Center, Hampton, Virginia, with Dr. Aaron Goldman (University of Denver) and Mr. James M. Hoell (Langley) acting as co-chairmen. A list of attendees is given in table I. The specific objectives of the Workshop were: (1) to review in detail the current status of experimental and theoretical spectroscopic data on atmospheric species, (2) to explore methods for disseminating new data in a format readily available for applications, and (3) to discuss formalization of the Workshop in order to support objectives (1) and (2) on a long term basis.

A major portion of the Workshop was devoted to discussing the status (i.e., accuracy and availability) of spectroscopic data currently available on stratospheric species. Table II lists the molecules that were considered. While this list is extensive, it is not meant to be complete. Table III is a summary of information assembled by the Workshop attendees related to research completed (C), underway (U), or planned (P) at a number of U.S. or foreign laboratories. Here again, the table is not complete, but provides a good review of the current status of the spectroscopic data available to the user community.

During the status review, the initial emphasis was placed on the spectral data available on the more abundant species (H_2O, O_3, CO_2, CH_4, and N_2O). This approach was selected since a large body of spectral data already exists for these molecules, and interfering effects from these species often represent the limiting factor on our ability to identify and quantify many of the less abundant species. It should be noted that this Workshop report does not explicitly enumerate the requirements imposed on spectral data by the various instruments or science missions. However, throughout the review process, instrument requirements and scientific goals were considered.

Specific recommendations for additional experimental and theoretical research are given below. In general, the recommendations reflect the feeling of the Workshop attendees that additional quantitative spectral data are needed on the species which have been detected and require more accurate atmospheric measurements, while only qualitative spectral data (i.e., location of absorption features) are needed for the extremely tenuous species which have not yet been detected in the stratosphere.

The discussions related to objective (2) centered around the continued use of the AFGL format for compiling spectroscopic parameters. Dr. L. Rothman, from AFGL, reviewed his current efforts and limitations for updating and expanding the AFGL line parameter tape. In summary, this is a continuing effort at AFGL, but is limited by the availability of data suitable for inclusion on the tape as well as manpower to evaluate, select, and format the data.

The recommendations relative to objectives (2) and (3) tend to be less specific than those associated with objective (1). This is due to the uncertainty in the degree of long range support that might eventually be available.

RECOMMENDATIONS

General

(1) Future meetings of the Workshop should be convened with representatives from other organizations and specialists on specific molecules.

(2) A newsletter should be established and mailed periodically to update and improve the data contained in table III and to solicit data for the AFGL compilation. The goal of the current Workshop should be expanded to provide a forum to aid in obtaining and reviewing spectroscopic data for the AFGL tape. However, such activities will require support from one or more government agencies.

(3) Most molecules require additional studies for more accurate determination of the effects of temperature and foreign gas broadening on spectral line widths along with high resolution measurements to determine far wing line shapes.

(4) For the major atmospheric species (i.e., CH_4, H_2O, CO_2, O_3, and N_2O) long path absorption measurements are needed to identify weak transitions.

SPECIFIC RECOMMENDATIONS

CH_4

(a) Since a sizeable body of experimental data is currently available for CH_4, a quantum mechanical analysis of CH_4 should be performed using the current data base.

(b) Additional long path absorption data are required for identification of weak lines (i.e., $\leq 10^{-26}$ cm per molecule).

(c) Experimental and analytical studies are required on the ν_4 band of the isotopic species of CH_4.

O_3

(a) Analysis of isotopic ozone is needed. The ν_3 isotopic band is particularly important because of its potential interfering effects.

(b) Line strengths for the $3\nu_3$, and $\nu_1 + \nu_2 + \nu_3$ are needed for the normal isotope of O_3.

N_2O

Measurements of the line intensities for the perpendicular bands are needed, as well as analysis of long path absorption data.

CO

Revised analysis of solar CO transitions is needed for the $\Delta V = 1$ and $\Delta V = 2$ bands.

H_2O

(a) Laboratory measurements for the ν_1, $2\nu_2$, and ν_2 band of HDO are needed.

(b) Measurements of line strengths for the high J transition are needed.

CO_2

(a) Additional CO_2 line position measurements are needed for vibrational energy levels above 2000 cm^{-1}.

(b) Analysis of long path absorption data is needed for identification of weak absorption lines.

(c) Additional laboratory studies are needed on line intensities in the 15 μm spectral region.

(d) Additional experimental and analytical work is needed on the 5 μm isotopic CO_2 band.

HCl

Experimental studies of half width versus temperature.

ClO

Experimental studies of half width versus temperature.

HF

Measurements of line intensities are needed at room temperature to verify extrapolated values obtained at 400 K.

HBr

Experimental values of half width are not available; however, current estimates are probably sufficient to support current atmospheric measurements.

HNO_3

Analysis of high resolution diode laser data and lower resolution spectra has provided line intensities, half width, and quantum assignments of the ν_5 band. However, additional diode laser measurements are needed in the 870 to 865 cm^{-1} region to check extrapolation of this analysis. Additional work is also needed for the R-region of the $2\nu_9$ band. Analysis of available high resolution data of the ν_3 and ν_4 region is needed. The ν_2 region analysis needs to be extended to the wings of the band.

HOCl

Pressure and temperature effects on half width will be needed if HOCl is to be observed in the atmosphere.

Freon-12

Analysis of currently available diode laser spectra of the ν_6 (1161 cm^{-1}) and ν_8 (923 cm^{-1}) bands should be pursued.

CF_4

Line parameters are needed for the ν_3 region.

NO_2

Line parameters are needed for the wings of the ν_3 and $\nu_3 + \nu_2 - \nu_2$ band.

$ClONO_2$

Analysis of currently available diode laser spectra should be pursued.

H_2O_2

Line intensities and assignments are needed for ν_6 band of H_2O_2.

HO_2

Line position and intensity data are needed.

CH_3Cl

Line parameters are needed for the 3 μm region.

NH_3

An extensive data base is currently available; however, a critical comparison of the various experimental and theoretical results is needed.

SUMMARY

As a result of the Workshop recommendations, plans are underway for establishing a periodic newsletter and holding at least one additional meeting of the Spectrascopic Workshop. The format for the newsletter is shown in table IV. It is anticipated that this will be mailed from AFGL at least once a year and will encourage more rapid inclusion of new data on the AFGL compilation tape. Planning is underway to hold the next Workshop during the Ohio State Spectroscopic Conference in June 1980, with Dr. John Shaw as the host chairman.

The review undertaken at the Langley Workshop and the resulting recommendations, while certainly not complete, have identified important areas of future research. Moreover, the recommendations of both the Silverthorne and this Workshop have identified the desirability of supporting periodic workshops to maintain an up-to-date review as well as to assist in the timely dissemination of new spectral data.

TABLE I.- WORKSHOP ATTENDEES

Dr. Gilbert Amat
Laboratoire de Physique Moleculaire
et D'Optique Atmospherique
C.N.R.S.
Batiment 220
Campus D'Orsay
91405 Orsay, France

Dr. A. Barbe
Laboratoire de Physique Moleculaire
Faculte des Sciences
B.P. 347
51062 Reims, France

Dr. Linda Brown
Jet Propulsion Laboratory
4800 Oak Grove Drive
Pasadena, CA 91103
(213) 354-6085

Dr. Chuck Chakerian
NASA/Ames Research Center
Moffett Field, CA 94035
(415) 965-5510

Dr. Roland Drayson
Research Activities Bldg.
University of Michigan
Ann Arbor, MI 48105
(313) 764-7210

Dr. Aaron Goldman
Department of Physics
University of Denver
Denver, CO 80208
(303) 753-2879

Dr. John Hillman
NASA/Goddard Space Flight Center
Greenbelt, MD 20771
(301) 344-8431

Mr. James Hoell
NASA/Langley Research Center
Hampton, VA 23665
(804) 827-2818

Dr. Virgil Kunde
NASA/Goddard Space Flight Center
Greenbelt, MD 20771
(301) 344-5693

Dr. Arthur Maki
Molecular Spectroscopy Division
Building 221, Room B-268
National Bureau of Standards
Washington, DC 20234

Dr. William G. Mankin
NCAR
P.O. Box 3000
Boulder, CO 80303
(303) 494-5151

Dr. Jae Park
Mail Stop 401A
NASA/Langley Research Center
Hampton, VA 23665
(804) 827-2576

Dr. Robert Rogowski
Mail Stop 283
NASA/Langley Research Center
Hampton, VA 23665
(804) 827-2819

Dr. Laurence Rothman
Infrared Physics Branch
Air Force Geophysics Laboratory
Hanscom Air Force Base, MA 01731
(617) 861-2336

Dr. James M. Russell III
Mail Stop 401A
NASA/Langley Research Center
Hampton, VA 23665
(804) 827-2576

Dr. John Shaw
Department of Physics
Ohio State University
174 W. 18th Avenue
Columbus, OH 43210
(614) 422-2707

TABLE I.- Concluded

Dr. Mary Ann H. Smith
Physics Department
College of William and Mary
Williamsburg, VA 23185
(804) 827-2576

Dr. Robert Toth
Code EBT-8
NASA Headquarters
Washington, DC 20546
(202) 755-8566

TABLE II.- ATMOSPHERIC SPECIES

CH_4	H_2O
N_2O	OH
NO_2	CH_3Cl
HO_2NO_2	OCS
NO_3	CO
N_2O_5	HF
NH_3	HCl
CCl_3F	CO_2
CCl_2F_2	CH_3F
O_3	H_2CO
HNO_3	HDO
ClO	CFClO
$ClONO_2$	CF_2O
HOCl	HONO
HO_2	HB_r
H_2O_2	CF_4
NO	

TABLE III.- SUMMARY OF MOLECULAR SPECTROSCOPIC PARAMETERS

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
CCl_2F_2 (Freon-12)	840-940 1080-1180 1070-1250	EOCOM @ 60 mK	Laboratory spectra	C		University of Denver (Goldman)
CCl_2F_2 (Freon-12)	1150-1173	Diode laser @ 1 mK	Laboratory spectra Absorption coefficient vs. T & P	C C	1 mK	Langley Research Center (Hoell)
CF_2	850-1100	Diode laser @ ~3 mK	Position Assignment	C U	~1 mK	Physical chemistry Univ. of Cambridge
CF_3	850-1100	Diode laser @ ~3 mK	Position Assignment	C U	~1 mK	Physical chemistry Univ. of Cambridge
CF_4	1200-1300	EOCOM @ 60 mK BOMEN @ 20 mK	Laboratory spectra	C		University of Denver (Goldman)
CF_3Cl (Freon-13)	1070-1250	EOCOM @ 60 mK	Laboratory spectra	C		University of Denver (Goldman)
CF_3Cl (Freon-13)	1235-1265 (Selected regions)	Diode laser	Laboratory spectra Analysis	C U	1 mK	Goddard Space Flight Center (Hillman)
$CFCl_3$ (Freon-11)	8-12 μm		Temperature dependence of 8-12 μm band	C		Ames Research Center (Silvaggiv)
$CFCl_3$ (Freon-11)	810-890 1060-6160	EOCOM @ 60 mK	Laboratory spectra	C		University of Denver (Goldman)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
$^{12}CH_4$	1200-2400	FTS @ 15 mK	Position Position $\nu_2+\nu_4-\nu_2$	C C P		JPL (Margolis)
$^{12}CH_4$ [b]	ν_2,ν_4	Calculation	Position Strength	C C		Orton/Rohrette
$^{12}CH_4$	2400-3200	FTS @ 15 mK	Compilation of 9000 lines Position Strength Assignment	 90% C 90% C 70% C		JPL (Toth/Brown)
$^{12}CH_4$	3900-4700 ($\nu_3+\nu_4$)	FTS @ 15 mK	Position Assignment	C C		JPL (Toth/Brown)
$^{12}CH_4$	1200-1280	Diode laser @ 0.5 mK	Position Strength	C U	1 mK 1-2%	Goddard Space Flight Center (Hillman)
$^{12}CH_4$	1100-1800	EOCOM @ 60 mK BOMEN @ 20 mK	Spectral atlas Spectral atlas	C P		University of Denver (Goldman) Ames (Boese)
$^{12}CH_4$	2940-2990	Diode laser (Doppler resolution)	Line broadening (0.1 - 0.5 torr) Intensities	U U	±0.7 mK	JRC - ISPRA (Restelli)

[a]C = Complete; U = Underway; P = in Progress.
[b]Available for next version of AFGL Atmospheric Absorption Line Parameters Compilation (from Glenn Orton).

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
$^{12}CH_4$	1305-1327	Diode laser @ 4 mK	10 lines measured Relative intensity Absolute intensity	 C C	 5% 5%	JRC - ISPRA (Restelli)
$^{12}CH_4$	1243.34-1377.83	0.1 mK	Absolute line intensities	C		University of Tennessee (Fox) from Ames Newsletter
$^{13}CH_4$	1200-2000	FTS @ 15 mK	Position Some ν_4 assignments	C ---		JPL (Toth/Brown)
$^{13}CH_4$	2400-3200 ($2\nu_4, \nu_2+\nu_4, \nu_3$)		Position Assignments	C C		JPL (Toth/Brown)
$^{13}CH_4$	3900-4700		Position Some $\nu_3+\nu_4$ assignments	C ---		JPL (Toth/Brown)
$^{13}CH_4$	1200-1270	Diode laser @ 0.1 mK	Position Strength	U U		Goddard Space Flight Center (Hillman)
CH_4	1213-1380	60 mK	Position Intensities Assignment	U U U	4 mK	ONERA (Battineau)
CH_4	2404-2730		Position Assignment Intensities	C C		Dijon Lab

[a] C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
CH_4	2700-3000		Position Assignment Intensities	C C		Dijon Lab & JPL
CH_4	1100-1800	60 mK	Position Assignment	C C		Dijon Lab & LUTZ
CH_4	5600-7100	12 mK	Position Assignment	C C	1 mK	Dijon Lab (J. P. Maillard)
CH_4	2700-3500	7 mK	Position Assignment	C C	1 mK	Dijon Lab
CH_4	6057-4700	5 mK	Position Assignment	C C	1 mK	Dijon Lab
CH_4	1213-1386	50 mK	Position Assignment	C C	5 mK	Dijon Lab
CH_4	7000-9300	12 mK	Position Assignment	C C	1 mK	Dijon Lab (J. P. Maillard)
CH_4	7000-9200	12 mK	Position Assignment Intensities	C C C		Dijon Lab (J. P. Maillard)
CH_4	3686-6386	5 mK	Position Assignment	C C	1 mK	Dijon Lab (J. P. Maillard)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
CH_4	2858-4394	5.5 mK	Position Assignment	C C	1 mK	Dijon Lab
CH_4	5500-7000 ($2\nu_3$)	10 mK	Position Assignment	C C	0.5 mK	Observatoire de Meudon (J. O. Maillard)
CH_4	3700-11000	FTS @ 420 mK	Laboratory spectra	C		University of Arizona (U. Fink) from Ames Newsletter
CH_4	1.1 µm	1 m grating Spectrometer @ 160-300 mK	Laboratory spectra Analysis	C U		Ames Research Center (Giver) from Ames Newsletter
CH_4	2600-3200	10 - 20 mK	Position Strength Assignment	C C U		Florida State University (Hunt) from Ames Newsletter
$\left.\begin{matrix} ^{13}CH_3D \\ ^{12}CH_3D \end{matrix}\right\}$	1750-2400 ν_2	FTS @ 5.5 mK	Position Strengths	C C	0.3 mK ±5%	Ames Research Center (Chackerian) L. Infrarouge (Guelochvili)
CH_3D	1200-2000	FTS @ 15 mK	Line list	C		JPL (Toth/Brown)
CH_3D	2400-3200	FTS @ 15 mK	Spectrum	C		JPL (Toth/Brown)

[a] C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
CH_3D	1033-1270 1270-1420	40 mK	Position Assignment Relative Strength	C C C		Ohio State (Rao) Orsay (Tarrago)
CH_3F	2400-3200	FTS @ 10 mK	Laboratory spectrum	C		JPL (Margolis)
CH_3Br	1200-3200	FTS @ 10 mK	Laboratory spectrum Analysis	C P		JPL (Toth/Brown)
CH_3Cl	670-770 950-1110 1300-1600	EOCOM @ 60 mK	Laboratory spectra	C		University of Denver (Goldman)
CH_3Cl	2400-3200	FTS	Position	C		JPL (Margolis)
CH_2Cl_2	1200-3200	FTS @ 10 mK	Laboratory spectrum Analysis	C P		JPL (Toth/Brown)
CH_2Cl_2	720-800 1240-1300	EOCOM @ 60 mK	Laboratory spectrum	C		University of Denver (Goldman)
ClO[b]	849.63-858.74 871.70-874.40	Diode laser @ 1 mK	Position Strength Assignment	C C C	10-50 mK 20%	Langley Research Center (R. Rogowski)
ClO[b]	796-880	Diode laser	Position Strength Assignment	C		JPL (Menzies)

[a]C = Complete; U = Underway; P = in Progress.

[b]Available for next version of AFGL Atmospheric Absorption Line Parameters Compilation (from Glenn Orton).

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
$ClONO_2$	1250-1330	60 mK	Position Intensity (curve of growth of Q branch @ 1292 cm^{-1})	C C		ONERA (Louisnard)
$ClONO_2$	1250-1350	EOCOM @ 60 mK BOMEN @ 20 mK	Laboratory spectrum	C		University of Denver (Goldman)
$ClONO_2$	776-793	Diode laser @ 1 mK	Position Intensity Halfwidth Assignment	U U U	±50 mK	Langley Research Center (Rogowski)
CO			Intensities of CO overtone up to 15th vibrational level Isotopic data	C		Ames (Chackerian)
CO	Pure rotation, fundamentals, and overtones AFGL data being updated Canadians have new data Goldman has data for $\Delta V = 1$ solar CO lines D. Williams - self- and foreign-gas broadening					

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
CO_2	1600-2400	FTS @ 6 mK	Position Strength	C U	2 mK	AFGL and U. Mass. (H. Sakai)
$^{13}CO_2$	2170-2335	30 mK	Position	C		Ohio State (Rao)
$^{13}CO_2$	4.3 μm	30 mK	Strength	C		Ohio State (Rao)
CO_2	800-4000	FTS @ 50 mK	Long path absorption spectral - analysis underway	U	1 mK	Ohio State (Shaw)
$^{12}CO_2$ $^{13}CO_2$	3700-7000	9 mK	Position Assignment	C C	0.2 mK	Télescope IR Obs.de Meudon (J. P. Maillard)
$^{12}CO_2$ $^{13}CO_2$	3400-8150	100 mK	Position Assignment	C C	80 mK	National Research Council (C. Courtey)
COF_2	730-830 1180-1280	EOCOM @ 60 mK	Laboratory spectrum	C		University of Denver (Goldman)
COF_2	1200-2200	FTS @ 10 mK	Laboratory spectrum Analysis	C P		JPL (Toth/Brown)
HF	HF, HCl, HI, and HB_r available from R. Tipping, University of Nebraska, and are being incorporated onto the AFGL Trace Gas Compilation.					
HBr	2500-2600		Position Intensity	C C	15%	University of Denver (Goldman)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
HCl	2770-3000	24 mK	Position Assignment	C C		Départment de Physique Atomique & Moléculaire Universite of Rennes (J. P. Haudeau)
HCl	2700-3000	24 mK	Position Assignment	C C		Universite de Rennes
H_2CO	1200-2700	FTS @ 10 mK	Laboratory spectrum	C		JPL (Toth/Brown)
H_2CO	1 - 15	MMW spectrometer @ Doppler limit	Position	C	5×10^{-7} cm^{-1}	Physikalisch Chemisches Institute Justus Liebig - Universität
HCHO	1760-1780	60 mK	Position Intensity (curve of growth @ 1764.96 cm^{-1})	C C		ONERA (Louisnard)
HNO_3	865-885	110 mK	Position Assignment Intensities	C C C		Spectroscopie Moleculaire (Lado-Bordawyky)
HNO_3	860-907	50 mK	Position Assignment	C	7 mK	ONERA/LPMOA (Giraudet-Chevillard)
HNO_3	1270-1370	60 mK	Position Intensities	C	3 mK	ONERA (Giraudet)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
HNO_3	1200-1350 1600-1800	BOMEN @ 20 mK	Laboratory spectra	C		University of Denver (Goldman)
HNO_3	840-940	EOCOM @ 60 mK	Laboratory spectra	C		University of Denver (Goldman)
HNO_3	850-870	Diode laser	Position Intensity	U U	±0.4 mK	National Bureau of Standards (Maki)
HNO_3	1670-1726	Diode laser	Position Intensity	C	±0.4 mK	National Bureau of Standards (Maki)
HNO_3[b]	1718.97-1729.57	Diode laser @ 1 mK	Position Intensity Halfwidth	C	10 mK	Langley Research Center (Bair)
HNO_3	891.25-898.77	Diode laser @ 1 mK	Position Intensity Halfwidth	C	5 mK	Langley Research Center (Bair)
HNO_2	1685-1727	Diode laser	Position Assignment Relative intensity	C C C	±4 mK	National Bureau of Standards (Maki)
HNO_3	700-1900	60 mK	Line intensities N_2 broadening	C C		U. Maryland (Wilkerson) Ames (Giver)

[a]C = Complete; U = Underway; P = in Progress.

[b]Available for next version of AFGL Atmospheric Absorption Line Parameters Compilation (from Glenn Orton).

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
HDO	2900-4000	FTS @ 15 mK	Position Strength	U		JPL (Toth)
HO_2	850-1100	Diode laser @ ~3 mK	Position Assignment	C	~1 mK	Physical Chemistry Univ. of Cambridge
HO_2	1100 cm^{-1} region	Laser	Intensity (few lines)	U		JPL (Toth/Brown)
$H_2{}^{16}O$ AFGL update	1600-2650 $\nu_2, 2\nu_2-\nu_2, \nu_1-\nu_2, \nu_3-\nu_2$	5 mK	Position Relative intensity Absolute intensity Assignment	C C C C	5 mK 10% 10%	LPMOA (Camy-Peyret, Flaud)
$H_2{}^{16}O$ AFGL update	2620-4500 $\nu_1, 2\nu_2, \nu_3$	5 mK	Position Assignment	C C	1 mK	LPMOA (Flaud, Camy-Peyret)
$H_2{}^{16}O$	4200-5000	70 mK	Position Relative intensity Absolute intensity Assignment	C C C C	5 mK 10% 15%	LPMOA (Camy-Peyret, Flaud)
$H_2{}^{16}O$	5000-6000	25 mK	Position Relative intensity Absolute intensity Assignment	C C C C	3 mK 8% 10%	LPMOA (Flaud, Camy-Peyret) JPL (Toth)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
$H_2{}^{16}O$	6000-78000	5 mK	Position Assignment	C C		LPMOA (Camy-Peyret, Flaud)
$H_2{}^{16}O$	7800-9400	70 mK	Position Assignment	C C		LPMOA (Flaud, Camy-Peyret, Rao)
$H_2{}^{16}O$	1580-2370 $\nu_2, 2\nu_2-\nu_2$	6 mK	Position Assignments Relative intensity	C P P	2 mK	AFGL (H. Sakai)
$H_2{}^{16}O$	7800-9400	70 mK	Position Assignments	C C		LPMOA (Flaud) Ohio State (Rao)
H_2O	13666-13987	50 mK	Line intensities N_2 broadening	C C		U. Maryland (Wilkerson) Ames (Giver)
H_2O	10407-10727	46 mK	Line intensities N_2 broadening	C C		Ames (Giver) U. Maryland (Wilkerson)
$H_2{}^{18}O$	2950-4200	FTS @ 10 mK	Position Strength	C C		JPL (Toth/Brown)
$H_2{}^{17}O$	2950-4200	FTS @ 10 mK	Position Strength	C C		JPL (Toth/Brown)
H_2O	800-4000	FTS @ 50 mK	Long path absorption spectra: Position Intensity Halfwidth	 U U U	10 mK	Ohio State (Shaw)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
H_2O	1500-2000	BOMEN @ 20 mK	Laboratory spectra	C		University of Denver (Goldman)
$H_2{}^{17}O$ $H_2{}^{18}O$	6974-7387	70 mK	Position Assignment	C C	5 mK	LPMOA (Flaud, Camy-Peyret) JPL (Toth)
$H_2{}^{17}O$ $H_2{}^{18}O$	5030-5640	50 mK	Position Assignment Relative intensity Absolute intensity	C C C	5 mK 8% 10%	LPMOA (Flaud, Camy-Peyret) JPL (Toth)
H_2O_2	1220-1277	Diode laser	Position	C	±1 mK	Goddard Space Flight Center (Hillman)
H_2O_2	3 μm region		Position Assignment	U U		Florida State Univ. (Brenda Young)
H_2O_2	1150-1350	BOMEN @ 20 mK	Laboratory spectrum	C		University of Denver (Goldman)
H_2O_2	1100-1400	60 mK	Intensities N_2 broadening $278 \leq T \leq 295$ K	P P		Ames (Valero)
HOCl	3250-3875	Grating	Position Intensity	C C		NBS (Wells)
HOCl	1200-1300	Diode Laser/ Grating	Position Relative intensity	C C		NBS (Sams)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
NF_2	850-1100	Diode laser @ ~3 mK	Position Assignment	C U	~1 mK	Physical Chemistry
NH_3	1200-2700	FTS @ 10 mK	Laboratory spectrum	C		JPL (Toth/Brown)
NH_3	750-950 1070-1210	EOCOM @ 60 mK	Laboratory spectrum	C		University of Denver (Goldman)
NH_2	11 μm region	CO_2 heterodyne technique	Position of 20 lines	C	1 mK	Goddard Space Flight Center (Hillman)
$^{14}N^{15}NO$	1800-6000	5 mK	Position Assignment	C C	1 mK	LPMOA (C. Amiot)
$^{15}N^{14}NO$	1800-6000	5 mK	Position Assignment	C C	1 mK	LPMOA (C. Amiot)
$^{14}N^{15}N^{16}O$	2100-2300	30 mK	Position	C	2 mK	Laboratory of Molecular Spectroscopy. NUMUR, Belgium (Courtoy/Blanquet)
$^{14}N^{14}N^{18}O$	2850-2950	30 mK	Assignment	C		
N_2O	522-627 1115-1300	Diode laser	Position Relative intensity Absolute intensity Halfwidth vs. pressure for few lines	C C U U	±10 mK	National Bureau of Standards (Maki)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
$^{14}N_2{}^{16}O$	1800-8090	5 mK	Position Assignment	C C	1 mK	LPMOA (C. Amiot)
$^{15}N_2{}^{16}O$	1800-6000	5 mK	Position Assignment	C	1 mK	LPMOA (C. Amiot)
$^{14}N_2{}^{18}O$	1800-3100	5 mK	Position Assignment	C	1 mK	LPMOA (C. Amiot)
N_2O	2400-3000		Position Line strength	C C		JPL (Toth/Brown)
N_2O	4000-4600		Pressure broadening @ RT	C		JPL (Toth/Brown)
N_2O	800-4000	FTS @ 50 mK	Long path Absorption spectra: Analysis $\begin{cases}\text{Position}\\ \text{Intensities}\\ \text{Half width}\end{cases}$	U	1 mK	Ohio State (Shaw)
N_2O	522-627	Diode laser	Position Relative intensities Absolute intensity Line widths vs. pressure	C C U U	±10 to 1 mK	National Bureau of Standards (Maki)
NO_2	1500-1700	BOMEN @ 20 mK	Laboratory spectra	C		University of Denver (Goldman)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
NO_2	2862-2940	FTS @ 10 mK	Strength Spin splitting	C C		JPL (Toth/Hunt)
NO_2	4680-4777	5 mK	Position Assignment	U U	1 mK	Spectroscopie Moléculaire (Dana)
NO_2	4120-4200	5 mK	Position Assignment	U U	1 mK	Spectroscopie Moléculaire (Dana)
NO_2	1588-1629	60 mK	Position Assignment Intensities	C C C	4 mK ±10%	ONERA - LPMOA (Fontanella-Dana)
NO_2	2900-2950	FTS @ 3 mK	Position Intensity	C U		Observatoire de Meudon (Maillard and Dana)
N_2O_4	1750	BOMEN	Band envelope	C	20 mk	University of Denver (Goldman)
N_2O_5	500-2000	FTS (Nicolet)	Band intensities	C	±10-20%	Ames Research Center (Lovejoy)
N_2O_5	1220-1270	EOCOM @ 60 mK BOMEN @ 20 mK	Laboratory spectrum	C		University of Denver (Goldman)
NO	1800-1960	EOCOM @ 60 mK	Laboratory spectra	C		University of Denver (Goldman)

[a] C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
NO	1700-2000	BOMEN @ 20 mK	Laboratory spectra	C		University of Denver (Goldman)
NO	1800-1900	24 mK	Position Assignment	U U		Universite de Rennes
$^{14}N^{16}O$ $^{15}N^{16}O$	1700-2200	2.7 mK	Position Relative intensities Assignment	C C C	1 mK	LPMOA (Amiot)
NO_2	1600-2200 3500-3800	70 mK	Position Relative intensities	U U		Universite de Rennes
O_3	700 (ν_2)		Position Relative intensity	C		Laboratoire de Physique Moléculaire-Reims (Barbe & Lille & Rao)
O_3	948-1215 ($\nu_3, \nu_2+\nu_3-\nu_2,$ $\nu_1+\nu_2-\nu_2,$ $2\nu_3-\nu_3,$ $\nu_1+\nu_3-\nu_1$)	10 mK	Position Intensity Assignment	C C C	2 mK 1%	Laboratoire de Physique Moléculaire-Reims (Barbe)
O_3	966-1234 (ν_1)	25 mK	Position Assignment	C C	4 mK	Laboratoire de Physique Moléculaire-Reims (Barbe)

[a]C = Complete; U = Underway; P = in Progress.

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
O_3	2900-3122	25 mK	Position Intensity Assignment	C U U	5 mK	Laboratoire de Physique Molécularie-Reims (Barbe)
O_3	2710-2804 $(\nu_1+\nu_2+\nu_3)$	25 mK	Position Intensities Assignment	C U U	5 mK 20% (absolute)	Laboratoire de Physique Moléculaire-Reims (Barbe)
O_3	1700-1850 $(\nu_2+\nu_3, \nu_1+\nu_2)$	15 mK	Position Assignment	C C	3 mK	Laboratoire de Physique Moléculaire-Reims (Barbe & LPMOA)
O_3[b]	948-1240 $\nu_3, \nu_1, \nu_2+\nu_3-\nu_2,$ $\nu_2+\nu_1-\nu_2, 2\nu_3-\nu_3$ $\nu_1+\nu_3-\nu_1$	Calculation $\simeq$3 mK	Position Assignment Intensity	C C C	3 mK 5-25%	LPMOA (Flaud, Camy-Peyret)
O_3	700 $\nu_2, 2\nu_2-\nu_2$	Diode laser @ 1 mK	Position Assignment	C C	2 mK	Rao, Flaud, Camy-Peyret
O_3[b]	1900-2250 $(2\nu_1, 2\nu_3, \nu_1+\nu_3)$	20 mK	Position Intensities Assignment	C C C	3 mK	Laboratoire de Physique Móleculaire-Reims (Barbe) LPMOA (Flaud, Camy-Peyret)
O_3	1038-1054 $(\nu_3, \nu_2+\nu_3-\nu_2)$	Heterodyne radiometer 5 MHz & 25 MHz	Position Relative strength	C U		Goddard Space Flight Center (Hillman)

[a]C = Complete; U = Underway; P = in Progress.

[b]Available for next version of AFGL Atmospheric Absorption Line Parameters Compilation (from Glenn Orton).

TABLE III.- Continued

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
O_3	800-4000	FTS @ 50 mK	Long path (100-1000 m) Absorption spectra: Analysis	 U	1 mK	Ohio State (Shaw)
O_3	1040-1049	Diode laser @ 1 mK	Position Relative intensities	C C	5 mK 10%	Langley Research Center (C. Bair)
O_3	3-40	50 mK	Position Intensities Assignment	C C C	±10 mK 1%	National Physical Labs. (George Chantry)
OCS	1020-1080 825-885 1655-1737	Diode laser; grating; heterodyne	Position Absolute intensity near 10 µm Relative intensity	C[b] C[b] C[b]	0.2-4 mK 10%	National Bureau of Standards (Maki) Harry Diamond Ordnance Laboratory
OCS	1000-2500	60 mK	Position Strength Halfwidth	C U U	10 mK <15%	NCAR (Drayson)
OCS	10 cm^{-1} - 20 cm^{-1}	MMW spectrometer @ Doppler limited	Position Assignment	C C	5×10^{-7} cm^{-1}	Physikulisch Chemisches Institut Justus Liehig - Universitüt Heirrich

[a]C = Complete; U = Underway; P = in Progress.
[b]Additional work in progress.

TABLE III.- Concluded

Molecule	Spectral coverage (cm^{-1})	Instrument and resolution	Type of data	Status (a)	Accuracy	Source
$^{16}O^{12}C^{34}S$ $^{16}O^{13}C^{34}S$	1950-2100	30 mK	Position Assignment	C C	2 mK	Spectroscopie Moléculaire NAMUR BELGIUM (Fayt)
SO_2	1123-1226	60 mK	Position Assignment	C C	4 mK	ONERA/LPMOA (Dana)
SO_2	1150-1172.5	Diode laser @ 0.1 mK	Position Assignment	C U		Langley Research Center (Hoell)

[a]C = Complete; U = Underway; P = in Progress.

TABLE IV.- HIGH RESOLUTION MOLECULAR SPECTROSCOPY RELEVANT TO ABSORPTION LINE PARAMETER COMPILATIONS

NAME(S):

AFFILIATION:

ADDRESS:

TELEPHONE: DATE:

MOLECULE:

WAVENUMBER RANGE:

INSTRUMENT:

RESOLUTION:

<u>EXPERIMENTAL CONDITIONS</u>

TEMPERATURE(S): PRESSURE(S):

PATHLENGTH: BROADENING GAS(ES):

<u>DATA FORMAT STATUS</u> (Indicate "Yes" or "No" in the blanks)

LINE POSITIONS: ______ ACCURACY:

RELATIVE INTENSITIES: ______

ABSOLUTE INTENSITIES: ______ ACCURACY:

HALFWIDTHS: ______

LINE ASSIGNMENTS: ______

AFGL FORMAT: ______ OTHER (SPECIFY):

ADDITIONAL COMMENTS:

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NASA CP-2136		

4. Title and Subtitle	5. Report Date
Review of Spectroscopic Data for Measurements of Stratospheric Species	June 1980
	6. Performing Organization Code
7. Author(s) Aaron Goldman and James Hoell, editors	8. Performing Organization Report No. L-13768
9. Performing Organization Name and Address NASA Langley Research Center Hampton, VA 23665	10. Work Unit No. 506-61-53-01
	11. Contract or Grant No.
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, DC 20546	13. Type of Report and Period Covered Conference Publication
	14. Sponsoring Agency Code

15. Supplementary Notes

Aaron Goldman: University of Denver, Denver, Colorado
James Hoell: Langley Research Center, Hampton, Virginia

16. Abstract

Results and recommendations from a two-day workshop conducted at Langley Research Center in October 1979 are discussed. A review of the current status of experimental and theoretical spectroscopic data on molecules of stratospheric interest is given along with recommendations for additional research. Methods for disseminating new and existing data are also discussed.

17. Key Words (Suggested by Author(s))	18. Distribution Statement
Spectroscopy Molecular parameters	Unclassified - Unlimited Subject Category 72

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price*
Unclassified	Unclassified	32	$4.50

*For sale by the National Technical Information Service, Springfield, Virginia 22161

NASA-Langley, 1980